# Simulation of Chemical Reactions in Big Volumes

**Reactant**

Temperature-dependent physical properties: specific heat, density, thermal conductivity

Chemical properties from *Kinetics Neo*: model-free / model-based parameters

**Container**

Shape, container material and thickness for each surface

*Different Surroundings*: heat transfer coefficient and emissivity for each surface

**Simulations**

For user-defined temperature program for each surface:

isothermal, dynamic, multiple steps, modulated, external temperature profile

**Visualization**

2D / 3D / Heatmap

for temperature, conversion, conversion rate, concentrations, $T_g$ for curing

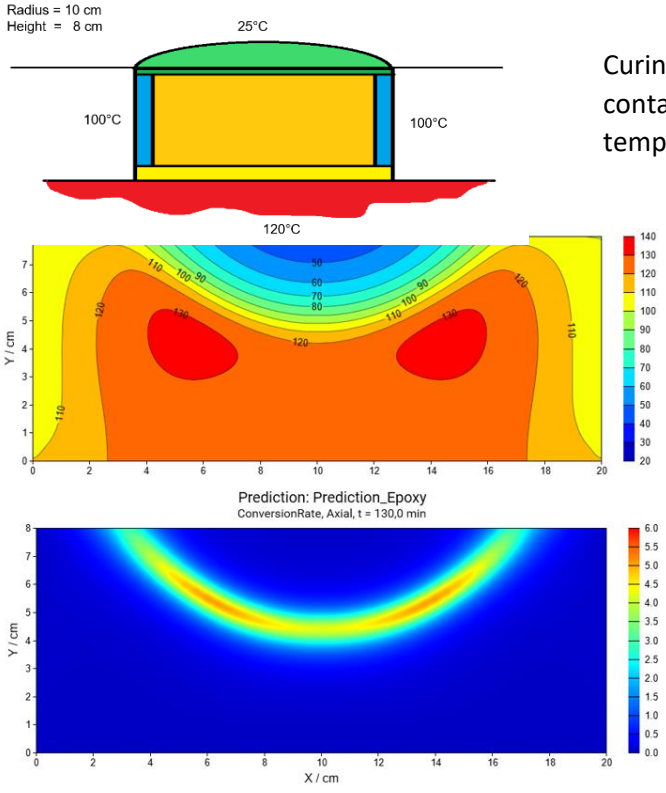
## *Termica Neo can:*

- Simulate your material behavior at each point in the container.
- Predict your degree of curing, decomposition, crystallization.
- Determine thermal safety conditions for production and storage.

## *Termica Neo answers the questions:*

- When and where is the maximal temperature?
- When and where is the maximal conversion rate?
- What are the temperature, conversion, and concentrations for a given time and position?

## *Curing in Cylindrical Container*




Curing of epoxy in cylindrical aluminum container with different container thicknesses (from 0.3 to 1 cm) and different temperature conditions on each surface.

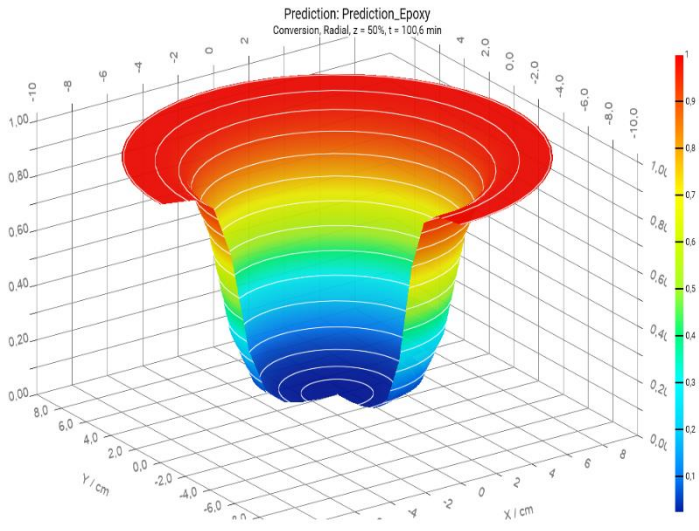



Fig. 1. Temperature and conversion rate for the vertical cross-section at a time of 130 min. Red areas on temperature plot are hot spots due to self-heating.

Fig. 2. Degree of conversion for the horizontal cross-section at 50% of sample height and a time of 100 min.

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## *Self-Acceleration Decomposition Temperature (SADT)*

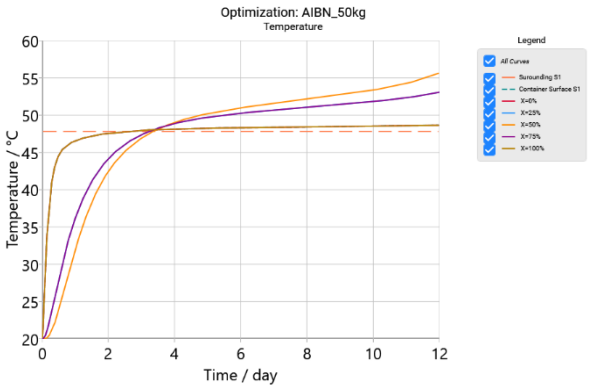


Fig. 4. SADT calculation for decomposition of the package of 50 kg AIBN

## *Reactant in Adiabatic Container*

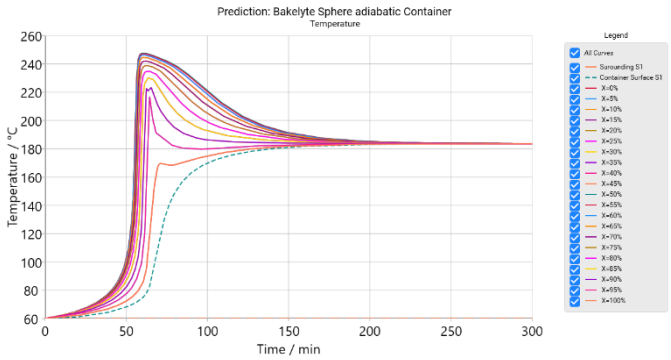


Fig. 5. Simulation of the temperature distribution of an adiabatic system: reactant (solid lines) in a container (dashed line).
The final temperature corresponds to the classical results calculated by using the Phi-factor.

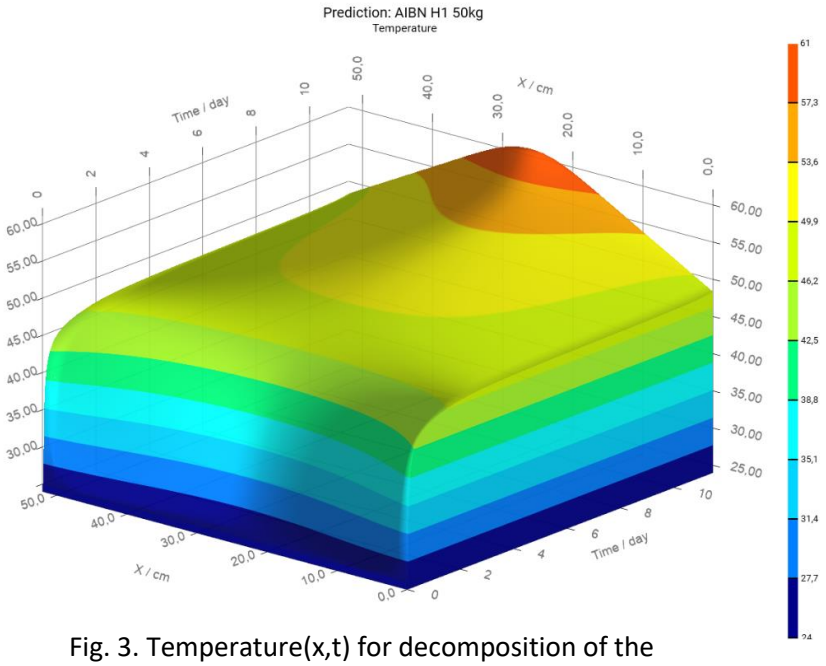


Fig. 3. Temperature(x,t) for decomposition of the package of 50 kg AIBN

## *What Makes Termica Neo So Valuable*

- Fast and easy-to-handle via user interface similar to Kinetics Neo
- The kinetic modes are taken directly from Kinetics Neo project (results of any method including both model-based and model-free)
- Calculation of the following properties at each point of volume as a function of time:
  - temperature
  - conversion
  - conversion rate
  - concentrations
  - glass transition temperature
- Calculation of Self-Accelerating Decomposition Temperature (SADT) with various materials, containers and surroundings
- Simulation of reactions for a reactor with container including adiabatic conditions


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